

Acetic acid

64-19-7 | DTXSID5024394

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2.40 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.42e-01

Confidence level: 6.10e-01

Nearest Neighbors from the Training Set

Image not found

Acetic acid

Measured: 1.00

Predicted: 2.40

Image not found

Acetamide

Measured: 5.01

Predicted: 4.44

Image not found

Acrylamide

Measured: 50.1

Predicted: 16.7

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Thioacetamide

Measured: 6.03

Predicted: 6.43

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Thiourea

Measured: 7.08

Predicted: 6.02